$$LogS = 0.92 - clogP*0.834 - MW*0.0084 \quad (8)$$

The performance of the ACD method was much worse and yielded RMSE=1.09. The performance of the ACD method is compared with the described method on Figures 1 and 2.

CLAIMS

What is claimed is:

1. A method of predicting solubility of a chemical compound comprising the steps of:
   a. identifying an electronically stored library of chemical molecules;
   b. building a computational model of a solid state of a molecule from said library by assembling a cluster of three or more copies of said molecule using a molecular mechanics method;
   c. computing energy, packing and interaction parameters from said model;
   d. computing other descriptors useful for predicting solubility of said molecule;
   e. repeating steps (b), (c) and (d) for every molecule from said library;
   f. building a solubility model using a quantitative method, which uses the parameters and descriptors computed in steps (c), (d) and (e);
   g. repeating steps (b), (c) and (d) for said compound;
   h. computing predicted solubility of said compound using said model and parameters and descriptors computed for said compound in steps (c), (d) and (e).

2. The method of claim 1, wherein step (b) includes copes of solvent molecules in addition to copies of said molecule.

3. The method of claim 1, wherein protonation state of copies of said molecule is dynamically recalculated during building a model of a solid state.

ABSTRACT OF THE DISCLOSURE

Descriptors of cohesive interactions in the solid state are calculated from a computational model of a solid state, i.e. from a small cluster of copies of the molecule of interest assembled using a molecular mechanics method. A model for predicting solubility is built using the cohesive interaction descriptors along with other descriptors useful for this purpose. Predicted solubility is computed for the compound of interest by computing the same descriptors and applying the solubility model. Explicit modeling of solid state

allows to more accurately characterize cohesive interactions in solids, hence, more accurately predict solubility.